First Gogny-Hartree-Fock-Bogoliubov Nuclear Mass Model

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We present the first Gogny-Hartree-Fock-Bogoliubov (HFB) model which reproduces nuclear masses with an accuracy comparable with the best mass formulas. In contrast with the Skyrme-HFB nuclear-mass models, an explicit and self-consistent account of all the quadrupole correlation energies are included within the 5D collective Hamiltonian approach. The final rms deviation with respect to the 2149 measured masses is 798 keV. In addition, the new Gogny force is shown to predict nuclear and neutron matter properties in agreement with microscopic calculations based on realistic two- and three-body forces.

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Astrophysical considerations require us to build nuclear-mass models that have as rigorous a footing as possible (see [1] for a review on the *r*-process nucleosynthesis and the importance of nuclear masses). In this way one might hope to be able to extrapolate from the mass data, which cluster fairly closely to the stability line, out towards the neutron-drip line, and make reliable estimates of the properties (including masses) of nuclei that are so neutron rich that there is no hope of measuring them in the foreseeable future. To this end, a series of nuclear-mass models have been developed on the basis of mean-field models. So far, only the nonrelativistic Hartree-Fock-Bogoliubov (HFB) method with Skyrme and contact-pairing forces, in which the force parameters are fitted to essentially all the experimental mass data, has led to competitive mass formulas with respect to the more traditional macroscopic-microscopic mass formula based on the liquid drop approach [2] or other global approaches [3] (the use of the term "mass formula" follows the usual designation of any semiempirical mass model that has been fitted to essentially all mass data and for which a complete mass table, running from one drip line to the other, has been constructed). The Skyrme-HFB approach, together with phenomenological Wigner terms and correction terms for the spurious collective energy, has proven its capacity to reproduce the 2149 experimental masses [4] with a root mean square (rms) deviation similar to or even better than the best dropletlike models [5,6]. Although the Skyrme-HFB method has opened a new era in the construction of mass formulas, it remains to be tested with respect to other microscopic approaches, like the relativistic mean-field model or with respect to finite-range interactions, such as the Gogny interaction. Furthermore, effects beyond mean field are known to affect predictions significantly [7] but have either been crudely approximated or totally neglected in the previous mass formulas.

In this Letter, we present the first mass formula obtained within the HFB framework with a Gogny interaction taking into account all the quadrupole correlations self-consistently and microscopically. Though the existing Gogny forces like D1S or D1N present global properties in agreement with most observables, they are not suited for an accurate estimate of nuclear masses [8]. In contrast to the Skyrme-HFB calculations which reach a 0.6–0.7 MeV rms deviation with respect to the bulk measured masses, existing Gogny interactions cannot predict masses with an rms better than typically 2 MeV. For this reason, a new Gogny force has been developed and fitted to all measured masses, keeping the additional constraint to provide reliable nuclear matter and neutron matter properties, but also radii, giant resonance, and fission properties. In addition, for the first time the quadrupole collective corrections are included in the mass formula by solving the collective Schrödinger equation with the 5-dimensional collective Hamiltonian (5DCH) [9].

The Gogny-HFB model.—The Gogny HFB model has been described in length in various publications (see Refs. [8,10,11] and references therein). In the present work, we use both an axially and a triaxially deformed HFB code to perform the calculations. These are written in terms of an expansion of the single-particle functions in a harmonic-oscillator basis. The triaxial code is used here to determine the quadrupole corrections to the total binding energy and the charge radius. These are estimated within the 5DCH model [9] by

$$\Delta E_{\rm quad} = E_{\rm MF} - E_{\rm BMF}, \tag{1}$$

where $E_{\rm MF}$ is the mean-field (MF) energy obtained in the axial symmetry approximation and $E_{\rm BMF}$ is the binding energy obtained beyond the mean-field (BMF) approximation, i.e., including the quadrupole corrections treated with the 5DCH model. Similarly, dynamical corrections are known to affect significantly the nuclear radius. The quadrupole correction to the charge radii is estimated by

$$\Delta r_{\rm quad} = \sqrt{r^2_{\rm BMF} - r^2_{\rm MF}}, \tag{2}$$

TABLE I. Values of the D1M interaction parameters.

i	W_i [MeV]	B_i [MeV]	H_i [MeV]	M_i [MeV]	μ_i [fm]
1	−12 797.57	14 048.85	−15 144.43	11 963.89	0.50
2	490.95	−752.27	675.12	−693.57	1.00
	t_0 [MeV fm^4]	x_0	α	W_{LS} [MeV fm^5]	
	1562.22	1	1/3	115.36	

TABLE II. INM parameters for D1M at equilibrium density ρ_0. G_0 and G_0' are the corresponding Landau parameters [12].

ρ_0 [fm^{-3}]	a_v [MeV]	J [MeV]	m^*/m	K_v [MeV]	G_0	G_0'
0.165	−16.026	28.554	0.746	225.0	−0.013	0.711

the final charge radius being estimated by $r_{\rm th}^2 = r_{\rm MF}^2 + \Delta r_{\rm quad}^2$. Note that the quadruple corrections are calculated for even-even nuclei only and interpolated from those for the others. For closed shell nuclei, the Gaussian overlap approximation used within the 5DCH approach gives erroneous negative corrections. For those nuclei, the correction is therefore set to zero.

The total binding energy reads $E_{\rm th} = E_{\rm axial} + \Delta E_{\rm quad} + \Delta E_\infty$ where in addition to the quadrupole correlations, an infinite-basis correction ΔE_∞ is introduced due to the limitation of the number of major shells included in the axially symmetric calculation. The same procedure as described in Ref. [10] is followed to estimate ΔE_∞. If the energy $E_{\rm axial}$ obtained with the axial code using $N \lesssim 14$ major shells can be determined within a reasonable computation time, this is not the case for both ΔE_∞ and $\Delta E_{\rm quad}$. Therefore, to avoid intractable calculations, the adjustment of the Gogny force parameters to reproduce at best the experimental masses is not performed by systematically calculating these correction terms. Instead, the computational scheme described below is followed.

Fitting strategy.—A mass fit entails that every nucleus that is included in the fit has to be calculated many times over. Making a direct fit with a deformed HF code to all of the more than 2000 measured masses imposes a very serious strain on one's computer facilities, so that in practice, a specific strategy needs to be followed, especially in view of the large number of free parameters (typically 14) and the many observables that need to be fitted. The Gogny effective nuclear interaction (plus spin-orbit term) is expressed [11] as

$$V(1,2) = \sum_{j=1,2} e^{-(\vec r_1-\vec r_2)^2/\mu_j^2}(W_j + B_jP_\sigma - H_jP_\tau - M_jP_\sigma P_\tau) + t_0(1+x_0P_\sigma)\delta(\vec r_1-\vec r_2) \times \left[\rho\left(\frac{\vec r_1+\vec r_2}{2}\right)\right]^\alpha + iW_{LS}\overleftarrow{\nabla}_{12}\delta(\vec r_1-\vec r_2) \times \vec\nabla_{12}.(\vec\sigma_1+\vec\sigma_2), \quad (3)$$

where P_σ (P_τ) is the two-body spin- (isospin-) exchange operator. From the 14 interaction parameters, it is possible to express [12] the parameters of symmetric infinite nuclear matter (INM) at the equilibrium density ρ_0 [or equivalently the Fermi momentum $k_F = (3/2\pi^2\rho_0)^{1/3}$], namely, the energy per nucleon a_v, the symmetry coefficient J, the effective mass m^*, and the incompressibility coefficient K_v. These five parameters are explicitly introduced in the fits instead of 5 of the Gogny force parameters. Starting from a trial force providing a first estimate of $\Delta E_{\rm quad}$ and ΔE_∞, the following 3-step reiterative procedure is adopted:

(i) The 5 INM parameters as well as the spin-orbit parameter W_{LS} are adjusted through an automatic optimization procedure to minimize the rms deviation with respect to experimental masses [4]; the 5 INM parameters are, however, kept within their corresponding experimental ranges [5,8].

(ii) The remaining parameters (only the α and x_0 parameters are kept fixed) are manually adjusted to optimize quantitatively the rms deviation with respect to known charge radii [13] (in practice, this corresponds essentially to a modification of k_F) and qualitatively to the energy density curves of the infinite neutron matter (to agree with the realistic calculation of [14]) and symmetric matter in the four spin-isospin channels to agree with [15]. Any modification at this stage is fed back into step (i) to ensure an optimum mass prediction.

(iii) As soon as an acceptable reproduction of all the above-mentioned observables is achieved, the $\Delta E_{\rm quad}$ and ΔE_∞ correction energies are reestimated and the new force is fed back into step (i). A new iteration cycle begins until all the conditions are properly fulfilled with one unique force.

Results.—The parameters of our final Gogny force, called D1M, are given in Table I and the corresponding INM parameters in Table II. The deviations between all the

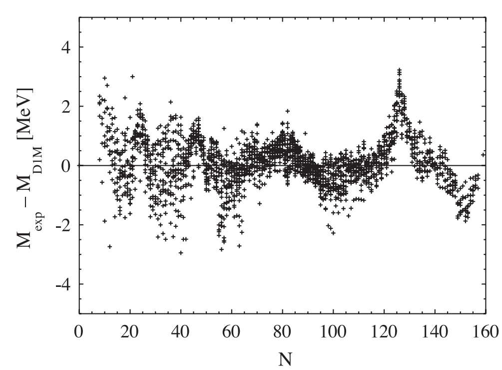

FIG. 1. Differences between measured [4] and D1M masses, as a function of the neutron number N.

TABLE III. rms (σ) and mean ($\bar{\epsilon}$) deviations between data and D1M predictions (energies in MeV, radii in fm).

	σ	$\bar{\epsilon}$
2149 masses [4]	0.798	0.126
2000 masses with $\lvert N-Z\rvert > 2$ [4]	0.771	0.155
1988 neutron binding energies [4]	0.538	0.004
1868 β-decay energies [4]	0.657	0.015
707 charge radii [13]	0.031	−0.008

2149 measured masses and the new D1M predictions are shown graphically in Fig. 1.

The rms values of these deviations are given in Table III. In particular, the rms deviation on masses amounts to 0.798 MeV, i.e., an accuracy comparable to the best available nuclear-mass formulas and by far better than the one obtained with previous Gogny forces. It should be noted that in the present calculation, no Wigner correction has been included.

If we only consider the 2000 nuclei with $|N-Z|>2$, the rms deviation is 0.771 MeV. As shown in Fig. 1, no deviation exceeds 3.2 MeV. However, as in all Skyrme-HFB mass formulas, the highest deviations occur around magic numbers, in particular, masses in the $N \simeq 126$ region remain significantly overbound. The inclusion of the particle-vibration coupling effects, known to modify the single-particle level density at the Fermi energy and consequently the amplitude of the shell effect, could change this trend.

The quadrupole correction energies obtained self-consistently with D1M are shown graphically in Fig. 2 and compared with those of D1N. They amount to no more than 5 MeV, but remain sensitive to the interaction, in particular, to the pairing strength and the effective mass. The quadrupole corrections obtained with different interactions (Fig. 2) typically affect the rms deviation by a few hundred keVs. This remains relatively large with respect to the mass model accuracy, so that it is mandatory to recalculate self-consistently the corrections at the end of a fitting iteration.

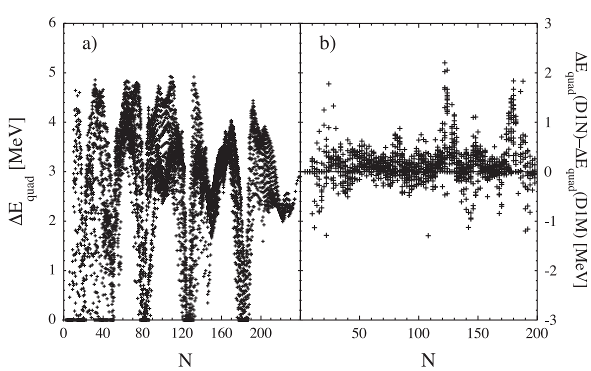

FIG. 2. (a) D1M quadrupole correction energies as a function of the neutron number for all nuclei considered here. (b) Difference between the quadrupole energies obtained with D1N and D1M for even-even nuclei with $N \leq 200$.

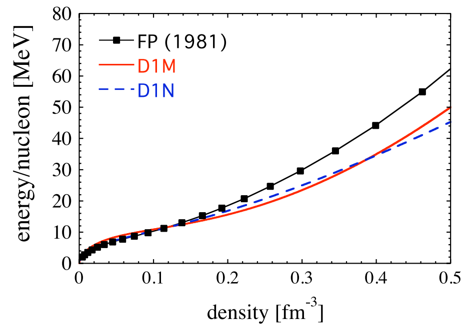

FIG. 3 (color online). Energy per neutron as a function of neutron matter density for D1N (dashed line), D1M (solid line), and for the calculations of Ref. [14] (FP; symbols).

As shown in Fig. 3, the neutron matter equation of state obtained with D1M is in close agreement, both with the D1N prediction and the realistic calculation of Friedman-Phandharipande (FP) [14] considered here as the reference curve.

Similarly, Fig. 4 shows the potential energy per particle for symmetric nuclear matter in each of the four two-body spin-isospin (S, T) channels for both D1M and Brueckner-Hartree-Fock (BHF) calculations with realistic two- and three-nucleon forces [15]. Note that the BHF calculations are still affected by non-negligible uncertainties (see, for example, [16]), so that only qualitative conclusions from such a global comparison of the interaction can be drawn. In this respect, a fair agreement between D1M and the realistic calculations can be seen in all states, in particular, the repulsive nature of the ($S=0$, $T=0$) state that is usually not reproduced by effective Skyrme interactions [16]. However, a different density dependence is found in the even-singlet ($S=0$, $T=1$) channel which is constrained by the pairing. In contrast to D1N predictions, we obtain with D1M the correct sign for the isovector splitting of the effective mass for neutron-rich matter, i.e., a higher neutron than proton effective mass $m_n^* > m_p^*$

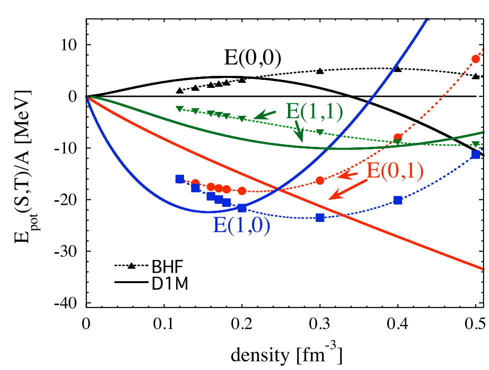

FIG. 4 (color online). Potential energy per particle in each (S, T) channel for BHF calculations [15] and D1M as a function of density for symmetric infinite nuclear matter.

TABLE IV. ^{208}Pb giant monopole (GMR), dipole (GDR), and quadrupole (GQR) resonance energies (in MeV) compared with experimental data for D1S, D1N, and D1M.

	D1S	D1N	D1M	Exp.
GMR	13.37	14.18	14.25	14.17 [18]
GDR	16.37	14.50	15.85	13.43 [19]
GQR	11.98	11.99	12.14	10.60 [20]

at all positive asymmetries. Such an isovector splitting of the effective mass is consistent with measurements of isovector giant resonances [16], and confirmed in several many-body calculations with realistic forces [17].

The new D1M force has also been tested with respect to various additional observables, such as the kinetic moment of inertia in Er or Pu nuclei, the giant monopole, dipole, and quadrupole energy in ^{208}Pb derived within the random-phase approximation (see Table IV), and the energy of the lowest 2^+ levels for the 519 even-even nuclei for which experimental data are available [21]. For all these observables, D1M and D1N give very similar results.

We have constructed a complete mass table including all nuclei in the range Z and $N \geq 8$ and $Z \leq 110$ located between the proton and neutron-drip lines. In Fig. 5, we compare these predictions with those of the "best-fit" Skyrme-HFB model (HFB-17) [6] and of the finite-range droplet model (FRDM) [2]. In both cases we see that despite the close similarity in the quality of the fits to the data given by these different models, large differences can emerge, especially for heavy nuclei ($Z > 80$) and as the neutron-drip line is approached ($N > 160$).

Conclusions.—We have described the first Gogny-HFB nuclear-mass model based on the D1M interaction. The rms deviation with respect to essentially all the available mass data has been reduced from typically a few MeV with previous interactions to less than 0.8 MeV. Furthermore, for the first time, the mass formula takes an explicit and self-consistent account of all the quadrupole correlations affecting the binding energy. The quadrupole corrections are estimated microscopically on the basis of a 5-dimensional collective Hamiltonian with the same D1M interaction. Given also the constraint imposed on the Gogny force by microscopic calculations of neutron matter and symmetric nuclear matter, this new model is particularly well adapted to astrophysical applications such as the r process of nucleosynthesis. Different improvements to the mass model should still be brought, in particular, including octupole correlations or generalizing the Gogny force by introducing a finite range to the density-dependent term [12].

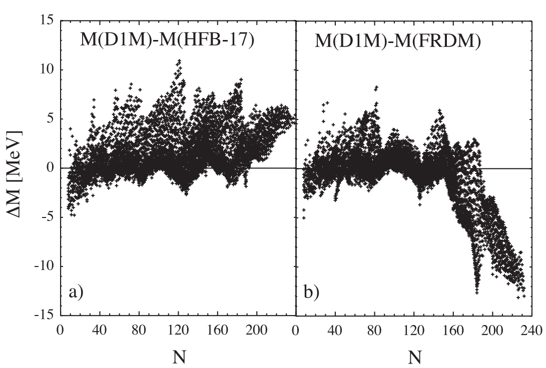

FIG. 5. Differences between (a) D1M and HFB-17 [6] masses and (b) D1M and FRDM [2] masses for all Z, $N \geq 8$, $Z \leq 100$ nuclei between the proton and neutron-drip lines.

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